FIG. 1

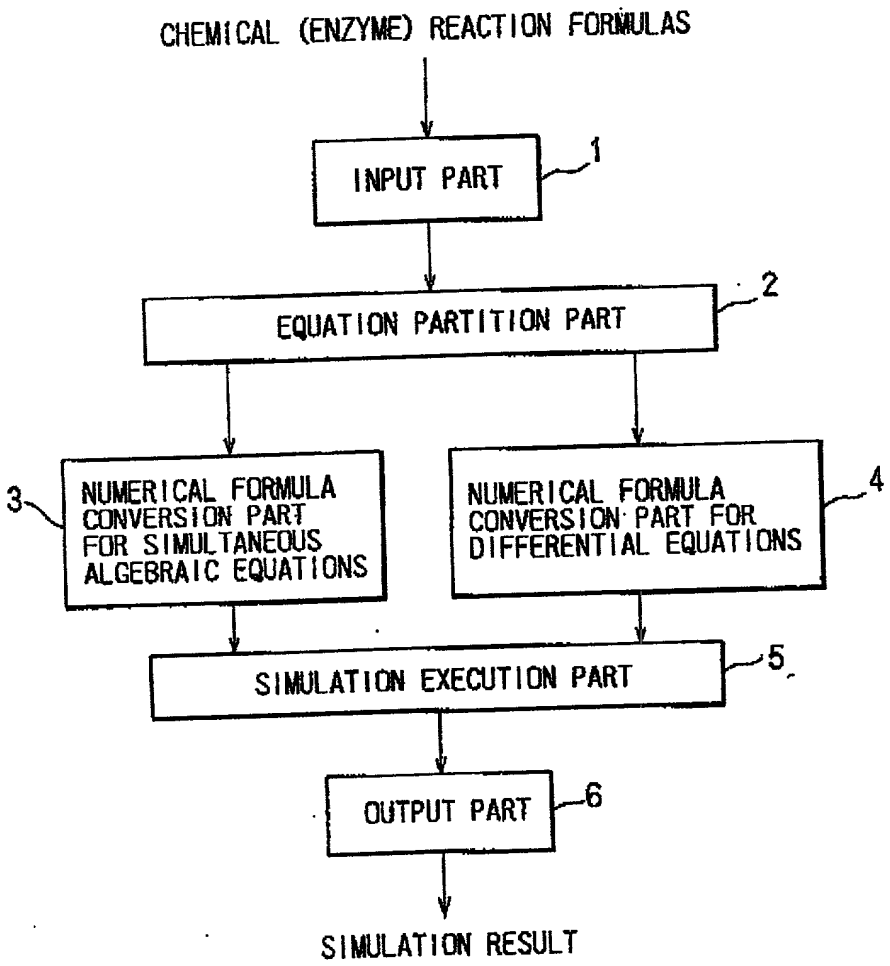

CHEMICAL (ENZYME) REACTION FORMULAS
INPUT PART
1
EQUATION PARTITION PART
2
NUMERICAL FORMULA CONVERSION PART FOR SIMULTANEOUS ALGEBRAIC EQUATIONS
3
NUMERICAL FORMULA CONVERSION PART FOR DIFFERENTIAL EQUATIONS
4
SIMULATION EXECUTION PART
5
OUTPUT PART
6
SIMULATION RESULT

FIG. 2

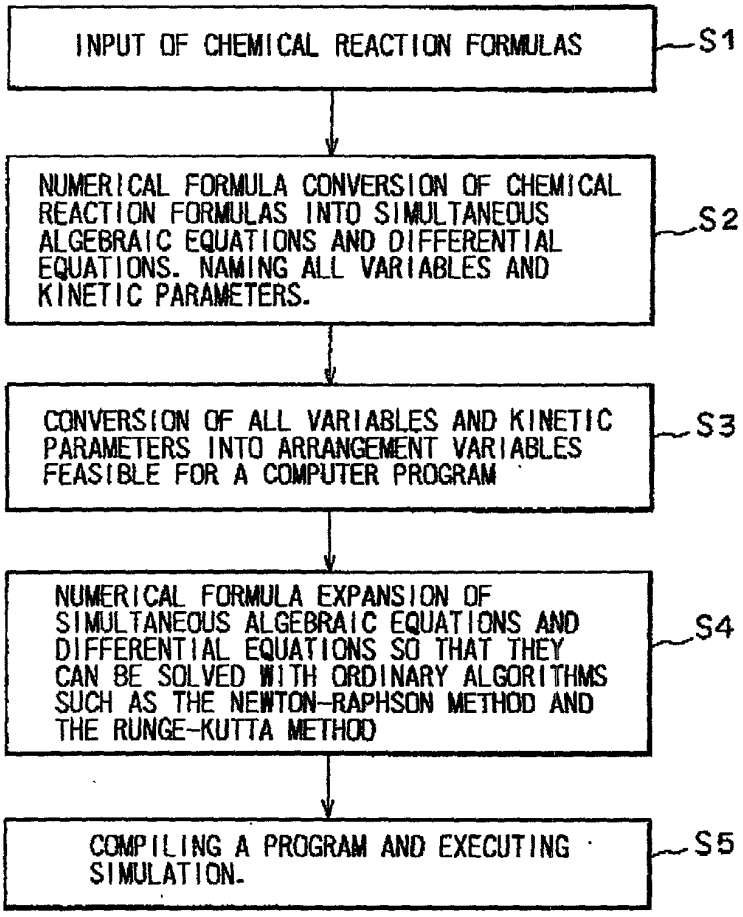

INPUT OF CHEMICAL REACTION FORMULAS
S1
NUMERICAL FORMULA CONVERSION OF CHEMICAL REACTION FORMULAS INTO SIMULTANEOUS ALGEBRAIC EQUATIONS AND DIFFERENTIAL EQUATIONS. NAMING ALL VARIABLES AND KINETIC PARAMETERS.
S2
CONVERSION OF ALL VARIABLES AND KINETIC PARAMETERS INTO ARRANGEMENT VARIABLES FEASIBLE FOR A COMPUTER PROGRAM
S3
NUMERICAL FORMULA EXPANSION OF SIMULTANEOUS ALGEBRAIC EQUATIONS AND DIFFERENTIAL EQUATIONS SO THAT THEY CAN BE SOLVED WITH ORDINARY ALGORITHMS SUCH AS THE NEWTON-RAPHSON METHOD AND THE RUNGE-KUTTA METHOD
S4
COMPILING A PROGRAM AND EXECUTING SIMULATION.
S5

FIG. 3

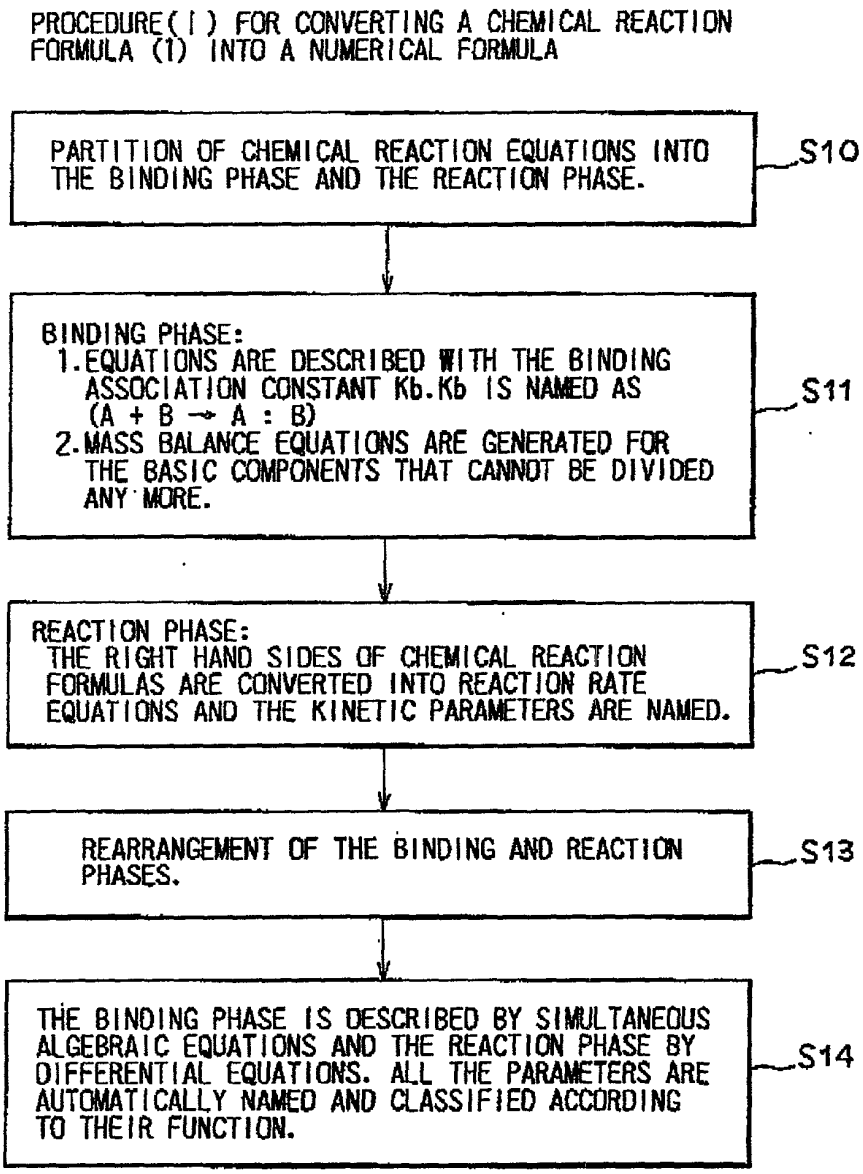

PROCEDURE(I) FOR CONVERTING A CHEMICAL REACTION FORMULA (1) INTO A NUMERICAL FORMULA
PARTITION OF CHEMICAL REACTION EQUATIONS INTO THE BINDING PHASE AND THE REACTION PHASE.
S10
BINDING PHASE:
1. EQUATIONS ARE DESCRIBED WITH THE BINDING ASSOCIATION CONSTANT Kb. Kb IS NAMED AS (A + B → A : B)
2. MASS BALANCE EQUATIONS ARE GENERATED FOR THE BASIC COMPONENTS THAT CANNOT BE DIVIDED ANY MORE.
S11
REACTION PHASE:
THE RIGHT HAND SIDES OF CHEMICAL REACTION FORMULAS ARE CONVERTED INTO REACTION RATE EQUATIONS AND THE KINETIC PARAMETERS ARE NAMED.
S12
REARRANGEMENT OF THE BINDING AND REACTION PHASES.
S13
THE BINDING PHASE IS DESCRIBED BY SIMULTANEOUS ALGEBRAIC EQUATIONS AND THE REACTION PHASE BY DIFFERENTIAL EQUATIONS. ALL THE PARAMETERS ARE AUTOMATICALLY NAMED AND CLASSIFIED ACCORDING TO THEIR FUNCTION.
S14

FIG. 4

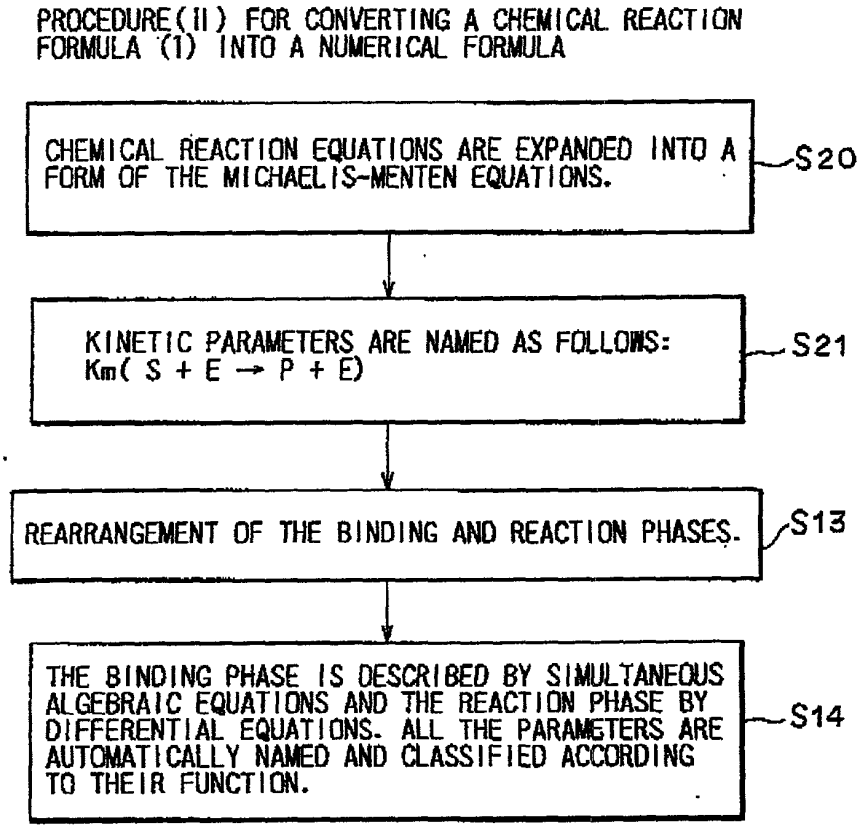
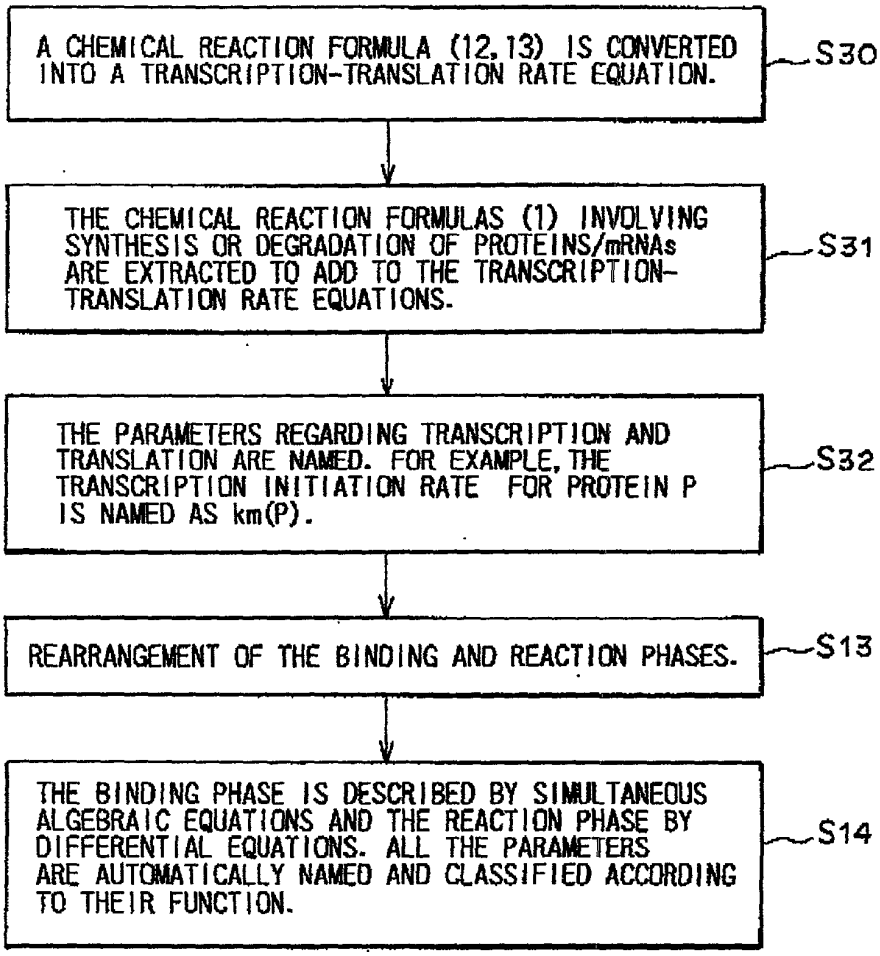

PROCEDURE(II) FOR CONVERTING A CHEMICAL REACTION FORMULA (1) INTO A NUMERICAL FORMULA
CHEMICAL REACTION EQUATIONS ARE EXPANDED INTO A FORM OF THE MICHAELIS-MENTEN EQUATIONS.
S20
KINETIC PARAMETERS ARE NAMED AS FOLLOWS:
Km(S + E → P + E)
S21
REARRANGEMENT OF THE BINDING AND REACTION PHASES.
S13
THE BINDING PHASE IS DESCRIBED BY SIMULTANEOUS ALGEBRAIC EQUATIONS AND THE REACTION PHASE BY DIFFERENTIAL EQUATIONS. ALL THE PARAMETERS ARE AUTOMATICALLY NAMED AND CLASSIFIED ACCORDING TO THEIR FUNCTION.
S14

FIG. 5

PROCEDURE OF CONVERTING CHEMICAL REACTION FORMULAS (1, 12, 13) INTO NUMERICAL FORMULAS.